

10/539,151

STN Structure

01/16/2008

Connecting via Winsock to STN

Search (Registry/Caplus)

Compd Clsins 20,23,32,36,41

Welcome to STN International! Enter x:x

LOGINID:SSPTAJMN1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 AUG 06 CAS REGISTRY enhanced with new experimental property tags
NEWS 3 AUG 06 FSTA enhanced with new thesaurus edition
NEWS 4 AUG 13 CA/CAPlus enhanced with additional kind codes for granted patents
NEWS 5 AUG 20 CA/CAPlus enhanced with CAS indexing in pre-1907 records
NEWS 6 AUG 27 Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 7 AUG 27 USPATOLD now available on STN
NEWS 8 AUG 28 CAS REGISTRY enhanced with additional experimental spectral property data
NEWS 9 SEP 07 STN AnaVist, Version 2.0, now available with Derwent World Patents Index
NEWS 10 SEP 13 FORIS renamed to SOFIS
NEWS 11 SEP 13 INPADOCDB enhanced with monthly SDI frequency
NEWS 12 SEP 17 CA/CAPlus enhanced with printed CA page images from 1967-1998
NEWS 13 SEP 17 CAPlus coverage extended to include traditional medicine patents
NEWS 14 SEP 24 EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS 15 OCT 02 CA/CAPlus enhanced with pre-1907 records from Chemisches Zentralblatt
NEWS 16 OCT 19 BEILSTEIN updated with new compounds
NEWS 17 NOV 15 Derwent Indian patent publication number format enhanced
NEWS 18 NOV 19 WPIX enhanced with XML display format
NEWS 19 NOV 30 ICSD reloaded with enhancements
NEWS 20 DEC 04 LINPADOCDB now available on STN
NEWS 21 DEC 14 BEILSTEIN pricing structure to change
NEWS 22 DEC 17 USPATOLD added to additional database clusters
NEWS 23 DEC 17 IMSDRUGCONF removed from database clusters and STN
NEWS 24 DEC 17 DGENE now includes more than 10 million sequences
NEWS 25 DEC 17 TOXCENTER enhanced with 2008 MeSH vocabulary in MEDLINE segment
NEWS 26 DEC 17 MEDLINE and LMEMLINE updated with 2008 MeSH vocabulary
NEWS 27 DEC 17 CA/CAPlus enhanced with new custom IPC display formats
NEWS 28 DEC 17 STN Viewer enhanced with full-text patent content from USPATOLD
NEWS 29 JAN 02 STN pricing information for 2008 now available

NEWS EXPRESS 19 SEPTEMBER 2007: CURRENT WINDOWS VERSION IS V8.2, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 11:29:29 ON 16 JAN 2008

=> fil reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 11:29:38 ON 16 JAN 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 JAN 2008 HIGHEST RN 1000000-66-7

DICTIONARY FILE UPDATES: 15 JAN 2008 HIGHEST RN 1000000-66-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

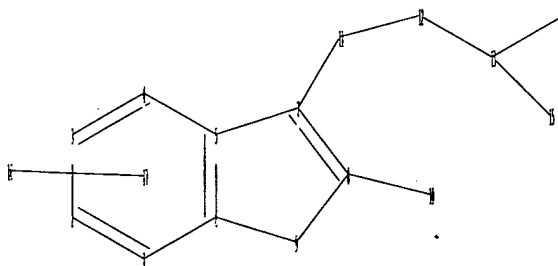
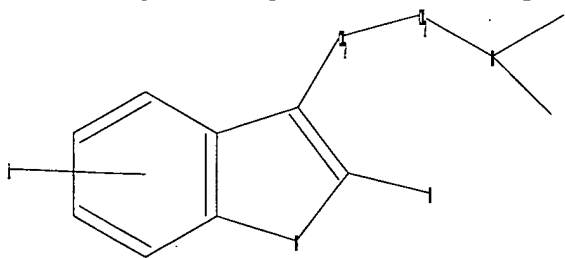
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10539151\Jan1.str



chain nodes :

10 11 12 16
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 14 15
chain bonds :
7-11 8-10 11-12 12-13
ring/chain bonds :
13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15
exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :

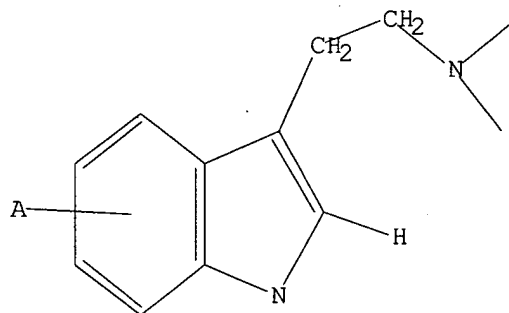
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



20

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 11:29:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 17947 TO ITERATE

11.1% PROCESSED 2000 ITERATIONS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

40 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 350918 TO 366962
PROJECTED ANSWERS: 6042 TO 8314

=> s 11 full ✓
FULL SEARCH INITIATED 11:30:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 356284 TO ITERATE

100.0% PROCESSED ✓ 356284 ITERATIONS
SEARCH TIME: 00.00.02

5875 ANSWERS

L3 5875 SEA SSS FUL L1

=> fil caplus
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
178.36	178.57

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 11:30:27 ON 16 JAN 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 16 Jan 2008 VOL 148 ISS 3
FILE LAST UPDATED: 15 Jan 2008 (20080115/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

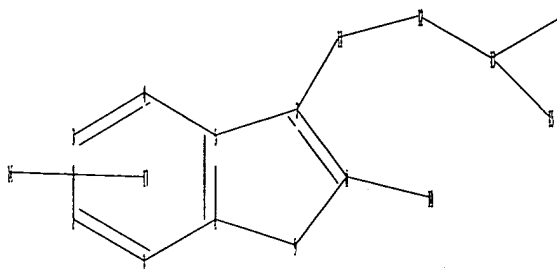
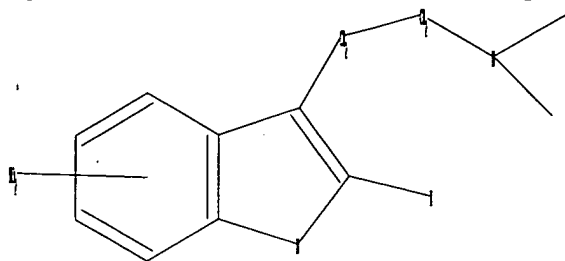
<http://www.cas.org/infopolicy.html>

=> s 13
L4 4163 L3

=> d ibib abs hitstr 4163

=>

Uploading C:\Program Files\Stnexp\Queries\10539151\Jan2.str



```

chain nodes :
10 11 12 16
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 14 15
chain bonds :
7-11 8-10 11-12 12-13
ring/chain bonds :
13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15
exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

```

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

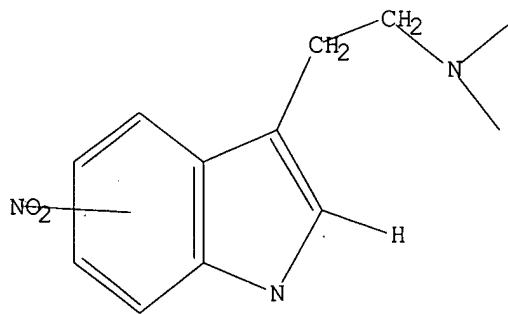
```

L5 STRUCTURE UPLOADED

=> d

L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15 full sub=13 ✓

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 11:32:51 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 246 TO ITERATE

100.0% PROCESSED 246 ITERATIONS
SEARCH TIME: 00.00.01

37 ANSWERS ✓

L6 37 SEA SUB=L3 SSS FUL L5

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH
L7 22 L6

=> d ibib abs hitstr 22

Claim 23

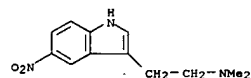
10/539,151

01/16/2008

L7 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 ACCESSION NUMBER: 1954:25005 CAPLUS
 DOCUMENT NUMBER: 48:25005
 ORIGINAL REFERENCE NO.: 48:4512a-1,4513a-e
 TITLE: The synthesis of nitro- and aminoindoles analogous to serotonin
 AUTHOR(S): Shaw, Elliott; Woolley, D. W.
 CORPORATE SOURCE: Rockefeller Inst. for Med. Research, New York, NY
 SOURCE: Journal of the American Chemical Society (1953), 75, 1877-81
 CODEN: JACSAT; ISSN: 0002-7863
 DOCUMENT TYPE: Journal
 LANGUAGE: Unavailable
 OTHER SOURCE(S): CASREACT 48:25005
 GI For diagram(s), see printed CA Issue.
 AB A series of new 3-alkyl- and 2,3-dialkylindoles has been prepared by the Fischer rearrangement. Aldehyde p-nitrophenylhydrazones have been converted with concentrated HCl in a biphasic system at room temperature to 3-alkyl-5-nitroindoles for the first time. A number of aminoindoles was readily prepared from the corresponding nitroindoles by reduction with Na2S2O4; other reducing agents led to mixts. The appropriate ketone p-nitrophenylhydrazones refluxed 3 h. with concentrated HCl (10 cc./g.) gave the corresponding indoles which were filtered off and washed with concentrated HCl and then with H2O. In this manner were prepared the following substituted 5-nitroindoles (substituents, % yield, and m.p. given): 2-Me, 3-Bu, 21, 125-6° (from C6H6-hexane); and 2-Me, 3-Cl(CH2)2, 32, 204-5° (from C6H6). The 2,3,3-tri-Me derivative, m. 124-5°, prepared in 48% yield by this method from p-O2NC6H4NHCH2CMe2 remained in solution and was precipitated by neutralizing the mixture. Crude 2-methyl-3-ethyl-5-nitroindole, prepared similarly, was purified by dissolving in boiling C6H6 (20 cc./g.), filtering, treating the filtrate near the b.p. with Al2O3 (1.5 g./1 g. crude base), evaporating the solution to 0.2 volume, and recrystg. the solid from EtOH to give the pure product, m. 190-1°. p-O2NC6H4NHCH2CMe2 (10 g.) was dissolved in a suspension of 5 g. p-O2NC6H4NHCH2CMe2 in 200 cc. concentrated HCl, a 200-mL layer of C6H6 added, the mixture stirred 3 h., the C6H6 replaced by fresh solvent, the mixture stirred again 3 h., the combined C6H6 layers were washed with H2O, dried with MgSO4, concentrated to about 25 cc., and the solution chromatographed on Al2O3 with C6H6 to yield 2.2 g. 3-ethyl-5-nitroindole, m. 94-5° (from C6H6-hexane), and, eluted with EtOH, 1.1 g. crystalline solid, m. 237-8°, apparently 1,1-bis(3-ethyl-5-nitro-2-indolyl)butane. The Et2O extract from a HIO4 cleavage of 245 g. isomeric chloropentadienols (cf. Paul and Tchelitcheff, C.A. 42, 4944f) was concentrated in vacuo 1 h., and the residue added to 100 g.

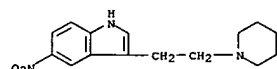
L7 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 p-O2NC6H4NHCH2CMe2 in 2 l. 50% AcOH to give 103 g. p-O2NC6H4NHCH2CMe2 (I), m. 101-2°. I (15 g.) stirred with two 750-cc. portions of C6H6 as described before, and the product resolved on Al2O3 gave 2.0 g. (15%) 3-(2-chloroethyl)-5-nitroindole (II), m. 120-1°; 5-[3-(2-hydroxyethyl)-5-nitroindole, m. 97-8°; 0.5 g. unidentified crystals, m. 134-5° (from C6H6-hexane); and 1.63 g. unidentified material, m. 82-3° (from aq. EtOH). II (1 g.) in 75 cc. EtOH let stand 10 days at room temp. With 50 cc. concd. NH4OH, the EtOH removed, the residual aq. suspension acidified with 6N HCl, filtered hot, and the filtrate treated slowly with alkali gave 0.63 g. (69%) 5-nitrotryptamine, m. 136-9°. II (1 g.) in 60 cc. EtOH let stand 4 days at room temp. with 40 cc. aq. 25% Me2NH, the EtOH removed in vacuo, and the pptd. base washed with H2O and treated with 6N HCl gave 57% 3-(2-dimethylaminoethyl)-5-nitroindole-HCl, m. 268-70° (from 95% EtOH). Similarly were prepd. the following analogous 3-substituted 5-nitroindole-HCl (substituent, % yield, and m.p. given): 2-piperidinoethyl, 51, 272-3° (from 95% EtOH); 2-(decahydro-1-quinolyl)ethyl, 10, 254-6° (from 95% EtOH); and 2-[[2-(4-imidazolyl)ethyl]amino]ethyl, dipicrate, 24%, 207-8° (from aq. Me2CO). 2-Methyl-3-(2-chloroethyl)-5-nitroindole (1.5 g.) in 75 cc. EtOH gave similarly with 30 cc. concd. NH4OH 75% 2-methyl-5-nitrotryptamine-HCl, m. 265-6°. In the same manner was obtained 88% 2-methyl-3-(2-piperidinoethyl)-5-nitroindole-HCl, m. 275-7° (from 95% EtOH). 2,3-Dimethyl-5-nitroindole (III) (3.8 g.) in 300 cc. PhMe distd. with 20 cc. M alc. EtOH until the b.p. of PhMe was reached, the residue refluxed, treated with excess MeI, filtered, the filtrate evapd. to dryness, and the residue chromatographed on Al2O3 with C6H6 gave 2.1 g. (51%) 1,2,3-trimethyl-5-nitroindole, m. 136-9° (from C6H6-hexane). III (0.85 g.) oxidized with 0.85 g. CrO3 in glacial AcOH and the crude oxidn. product hydrolyzed with aq. alc. HCl gave 0.22 g. ketone, needles, m. 148-50° (from aq. EtOH). III (5 g.) in 175 cc. EtOH and 100 cc. N NaOH treated at 50° with 25 g. Na2S2O4 in 120 cc. 0.5N NaOH, the almost colorless soln. filtered hot, the inorg. residue washed with EtOH, the alc. filtrate and washing concd. in vacuo, and the solid filtered off and recrystd. from EtOH gave 2.2 g. (52%) 2,3-dimethyl-5-aminoindole, m. 173-4° (from aq. EtOH). Similarly were prepd. the following aminoindoles (substituents, % yield, and m.p. given): 3-ethyl-5-amino (IV), 45, 116-18°; 2-Me deriv. (V) of IV, 64, 148-9°; 2-methyl-3-butyl-5-amino, 64, 96-8°; 2,3-dimethyl-4-amino (VI), 50, 156-60°; 2,3-dimethyl-6-amino (VII), 50, 117-18°; 2-methyl-3-ethyl-7-amino (VIII), 40, 110-12°; 1,2,3-trimethyl-5-amino, picrate, 41, 203-5° (from aq. EtOH); 3-(2-dimethylaminoethyl)-5-amino, dipicrate, 38, 202-4° (from H2O); 3-(2-piperidinoethyl)-5-amino, dipicrate, 67, 211-12° (from aq. EtOH); 2-methyl-3-(2-piperidinoethyl)-5-amino, 45, 149-51°; 5-aminoindole dipicrate, 60, 204-5° (from H2O); 2-methyl-5-aminoindole, 40, 112°; and 6-amino-1,2,3,4-tetrahydrocarbazole, 64, 146-7°. The UV absorption max. and min. in mμ and in parentheses, the corresponding ε × 10⁻³ values are for: 2-methyl-3-ethyl-4-nitroindole (IX), max. 240-5 (8.6),

L7 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 (inflection) (2.8), 408-12 (4.35), min. 295 (1.1); 5-NO2 isomer of IX, max. 276-7 (21.0), 336-7 (9.25), min. 240 (5.65), 305 (4.5); 6-NO2 isomer, max. 251 (9.1), 272 (6.2) 340-50 (7.1), 395-400 (9.25), min. 265 (5.9), 295 (2.3); 7-NO2 isomer, max. 240 (10.6), 259-60 (10.2), 372-8 (6.28), min. 250 (9.25), 300 (0.5); VI, max. 230 (31.0), 277-9 (6.8), min. 253 (3.6), 288-93 (6.05); V, max. 284-6 (6.84), 231-2 (24.7), min. 260 (3.74); VII, max. 235 (30.9), 273-5 (5.5), 307 (5.1), min. 255 (4.0), 290 (3.25); and VIII, max. 228 (35.8), 275-7 (8.5), 300 (inflection) (4.5), min. 250 (3.8). 2,3-Dimethyl-5-aminoindole (0.5 g.) and 0.32 g. OC(CH2)2CO.O heated 2 min. in an oil bath at 125°, the melt taken up in aq. Na2CO3, and the soln. gradually acidified gave 0.62 g. 2,3-dimethyl-5-succinimidindole, m. 147-9°; the mixt. heated longer gave 2,3-dimethyl-5-succinimidindole, m. 198-9°, insol. in aq. Na2CO3.
 IT 295796-33-7P, Indole, 3-(2-dimethylaminoethyl)-5-nitro-, hydrochloride 858828-08-7P, Piperidine, 1-[2-(5-nitro-3-indolyl)ethyl]- 860198-58-9P, Indole, 5-nitro-3-[2-(octahydro-1-(2H)-quinolyl)ethyl]-, hydrochloride 860359-59-7P, Indole, 5-nitro-3-(2-piperidinoethyl)-, hydrochloride
 RL: PREP (Preparation)
 (preparation of)
 RN 295796-33-7 CAPLUS
 CN 1H-Indole-3-ethanamine, N,N-dimethyl-5-nitro-, monohydrochloride (9CI) (CA INDEX NAME)



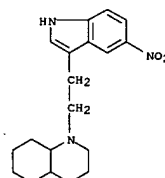
• HCl

RN 858828-08-7 CAPLUS
 CN Piperidine, 1-[2-(5-nitro-3-indolyl)ethyl]- (5CI) (CA INDEX NAME)



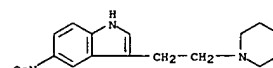
RN 860198-58-9 CAPLUS
 CN Quinolone, decahydro-1-[2-(5-nitro-3-indolyl)ethyl]-, hydrochloride (5CI) (CA INDEX NAME)

L7 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



• HCl

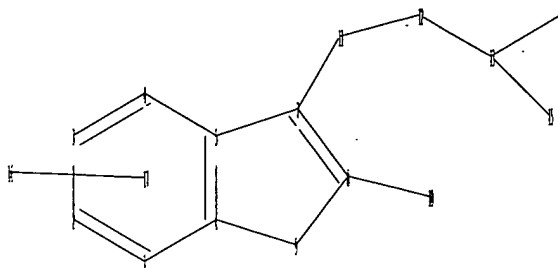
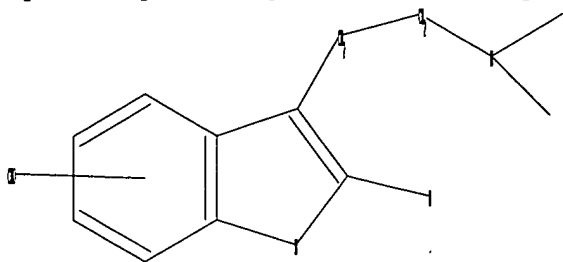
RN 860359-59-7 CAPLUS
 CN Indole, 5-nitro-3-(2-piperidinoethyl)-, hydrochloride (5CI) (CA INDEX NAME)



• HCl

=>

Uploading C:\Program Files\Stnexp\Queries\10539151\Jan3.str



```

chain nodes :
10 11 12 16
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 14 15
chain bonds :
7-11 8-10 11-12 12-13
ring/chain bonds :
13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15
exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

```

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:Atom

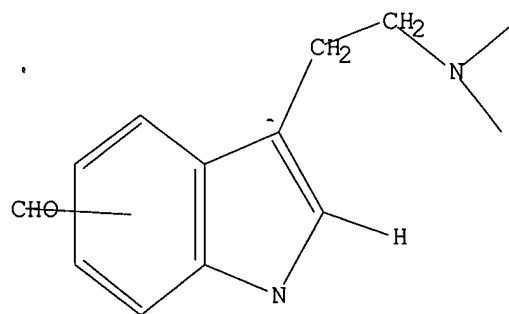
```

L8 STRUCTURE UPLOADED

=> d

L8 HAS NO ANSWERS

L8 STR



claim 32

Structure attributes must be viewed using STN Express query preparation.

=> s 18 full sub=l3

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 11:34:12 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 5875 TO ITERATE

100.0% PROCESSED 5875 ITERATIONS

SEARCH TIME: 00.00.01

10 ANSWERS

L9

10 SEA SUB=L3 SSS FUL L8

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH

L10 8 L9

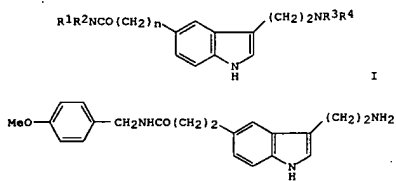
=> d ibib abs hitstr 8

L10 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:626347 CAPLUS
 DOCUMENT NUMBER: 105:226347
 ORIGINAL REFERENCE NO.: 105:36543a,36546a
 TITLE: Indole derivatives and pharmaceutical compositions containing them
 INVENTOR(S): Bays, David Edmund; Webb, Colin Frederick
 PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
 SOURCE: Ger. Offen., 60 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3543982	A1	19860619	DE 1985-3543982	19851212
BE 903846	A1	19860612	BE 1985-216004	19851212
SE 8505887	A	19860614	SE 1985-5887	19851212
GB 2169347	A	19860618	GB 1985-30591	19851212
GB 2169347	B	19880203		
AU 8551151	A	19860619	AU 1985-51151	19851212
AU 579687	B2	19881201		
FR 2574793	A1	19860620	FR 1985-18416	19851212
FR 2574793	B1	19881014		
NL 8503424	A	19860701	NL 1985-3424	19851212
JP 61151172	A	19860709	JP 1985-278124	19851212
ZA 8509520	A	19860827	ZA 1985-9520	19851212
CH 667454	A5	19881014	CH 1985-5301	19851212
			GB 1984-31426	A 19841213

PRIORITY APPLN. INFO.: CASREACT 105:226347; MARPAT 105:226347
 GI



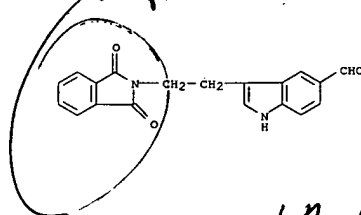
AB Indoles I [R1 = H, C1-6 alkyl, C3-7 cycloalkyl, C3-6 alkenyl, Ph or phenyl-C1-4-alkyl with Ph (un)substituted by C1-3 alkoxy, OH, halo, R5R6NCO (R5, R6 = H, C1-3 alkyl), R7R8N (R7, R8 = H, C1-3 alkyl; R7R8N = saturated monocyclic 5-7 membered ring); R2 = H, C1-6 alkyl; R1R2N = R7R8N;

L10 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

R3, R4 = H, C1-3 alkyl, 2-propenyl; n = 2-5] and their physiol. tolerable salts and solvates, useful as selective vasoconstrictors for cranial vessels at 0.5-50 mg, were prep. by 7 methods. 4-H2NOC6H4(CH2)2CO2H was diazotized and the product reduced with SnCl2 to give 4-H2NNHC6H4(CH2)2CO2H.HCl, which reacted with 2-(4,4-diethoxybutyl)-1H-isoindole-1,3(2H)-dione in refluxing aq. AcOH to give 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-1H-indole-5-propanoic acid. Successive reaction with pivaloyl chloride and 4-MeOC6H4CH2NH2 gave the N-[(4-methoxyphenyl)methyl]propanamide analog, hydrazinolysis of which gave indolylethylamine II, characterized as the hemisuccinate. Formulations for tablets, capsules, suppositories, and i.v. injection solns. were given.

IT 105323-64-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and Wittig reaction of)

RN 105323-64-6 CAPLUS
 CN 1H-Indole-5-carboxaldehyde, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]- (CA INDEX NAME)



phthal - proiv'60

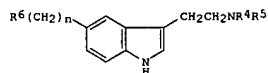
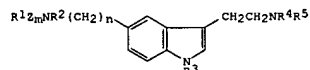
L10 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1987:575786 CAPLUS
 DOCUMENT NUMBER: 107:175786
 TITLE: Preparation of 5-(2-aminoethyl)tryptamines as
 antimigraine agents
 INVENTOR(S): Mills, Keith; Coates, Ian Harold; Bays, David Edmund;
 Webb, Colin Frederick; Dowle, Michael Dennis
 PATENT ASSIGNEE(S): Glaxo Group Ltd, UK
 SOURCE: Ger. Offen., 17 pp.
 CODEN: GWOXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3700407	A1	19870709	DE 1987-3700407	19870108
AU 8767418	A	19870709	AU 1987-67418	19870108
AU 597324	B2	19900531		
NL 8700027	A	19870803	NL 1987-27	19870108
GB 2186874	A	19870826	GB 1987-381	19870108
GB 2186874	B	19900207		
FR 2595352	A1	19870911	FR 1987-108	19870108
FR 2595352	B1	19900713		
JP 62228057	A	19871006	JP 1987-2590	19870108
AT 8700024	A	19871215	AT 1987-24	19870108
AT 386197	B	19880711		
ZA 8700104	A	19871230	ZA 1987-104	19870108
BE 1000072	A1	19880202	BE 1987-4	19870108
CH 671017	A5	19890731	CH 1987-46	19870108
			GB 1986-398	A 19860108

PRIORITY APPLN. INFO.:

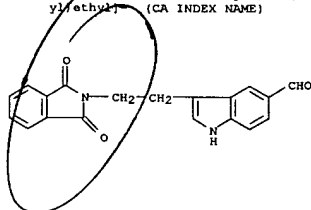
OTHER SOURCE(S): MARPAT 107:175786
 GI



AB The title compds. (I; R1 = H, C1-6 alkyl, C3-7 cycloalkyl, Ph, phenyl-C1-4 alkyl; R2, R3 = H, C1-3 alkyl; R4, R5 = CH2CH:CH2, R3: Z = CO, SO2; n = 2-5; m = 1) were prepared as antimigraine agents (no data).
 4-H2NNHC6H4CH2CN was refluxed with 4-phthalimidobutanal di-Et acetal in

L10 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

H2O/HOAc to give tryptamine II (NR4R5 = phthalimido, R6 = cyano, n = 1) which, on hydrogenation over PdO/C, gave II.HCl (NR4R5 = phthalimido, R6 = NH2, n = 2). This was stirred with Ac2O in pyridine and the product refluxed with H2NNH2 in EtOH to give II (R4 = R5 = H, R6 = AcNH, n = 2). Tablets were prepd. each contg. II (R4 = R5 = Me, R6 = 4-AcNHC6H4CH2CONH, n = 2) 2.4, CaHPO4 95.1, Croscarmellose Na 2.0, and Mg stearate 0.5 mg.
 IT 105323-64-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and Wittig reaction of)
 RN 105323-64-6 CAPLUS
 CN 1H-indole-5-carboxaldehyde, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)methyl] (CA INDEX NAME)



L10 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:107034 CAPLUS

DOCUMENT NUMBER: 120:107034

TITLE: Imidazole, triazole and tetrazole serotonin 5-HT1 receptor antagonists

INVENTOR(S): Castro, Pineiro Jose Luis; Matassa, Victor Giulio

PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK

SOURCE: PCT Int. Appl., 53 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9320066	A1	19931014	WO 1993-GB652	19930329
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9338956	A	19931108	AU 1993-38956	19930329
AU 675641	B2	19970213		
EP 637307	A1	19950208	EP 1993-907945	19930329
EP 637307	B1	20001108		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07505382	T	19950615	JP 1993-517223	19930329
JP 3285581	B2	20020527		
AT 197453	T	20001111	AT 1993-907945	19930329
ES 2152948	T3	20010216	ES 1993-907945	19930329
US 5607957	A	19970304	US 1994-313058	19940929
			GB 1992-7396	A 19920403
PRIORITY APPLN. INFO.:			WO 1993-GB652	A 19930329

OTHER SOURCE(S): MARPAT 120:107034
GI

AB The title compds. I [A1, A2 = H, hydrocarbon group, heterocyclic group, halogen, CN, CF3, (un)substituted amino, etc.; E = direct bond, (un)branched C1-4 alkylene; F = (un)substituted heterocyclyl; 2-4 of W, X, Y, and Z = N and the remainder are C; when W = X = Y = Z = N then A2 = nonbonded electron pair], which are serotonin 5-HT1 receptor antagonists (no data) and useful in the treatment of migraine headache (no data), are prepared and I-containing formulations presented. Thus, 3-[2-(dimethylamino)ethyl]-5-[(2-methyl-1,2,4-triazol-3-yl)aminomethyl]-1H-indole oxalate (m.p. 208-210°) was prepared from 2-methyl-3-nitro-1,2,4-triazole in 3 steps.

L10 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

IT 152673-51-3P 152673-52-4P

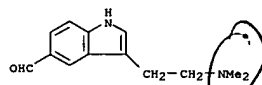
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of serotonin 5-HT1

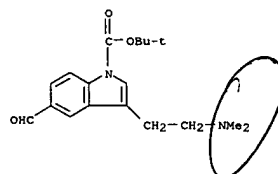
receptor antagonists)

RN 152673-51-3 CAPLUS

CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



RN 152673-52-4 CAPLUS
CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-5-formyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

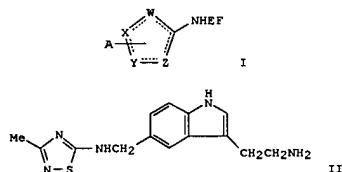


L10 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:245114 CAPLUS
 DOCUMENT NUMBER: 120:245114
 TITLE: Preparation of heteroaromatic 5-hydroxytryptamine receptor agonists
 INVENTOR(S): Castro Pineiro, Jose Luis; Matassa, Victor Giulio
 PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK
 SOURCE: PCT Int. Appl., 43 pp.
 CODEN: PFXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

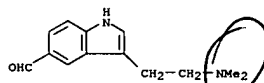
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9321182	A1	19931028	WO 1993-GB789	19930414
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9340766	A	19931118	AU 1993-40766	19930414
EP 636131	A1	19950201	EP 1993-910152	19930414
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07505649	T	19950622	JP 1993-518132	19930414
US 5510359	A	19960423	US 1994-318610	19941007
			GB 1992-8463	A 19920416
PRIORITY APPLN. INFO.:			WO 1993-GB789	A 19930414

OTHER SOURCE(S): MARPAT 120:245114
 GI

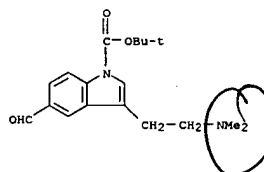


AB Title compds. I (W, X, Y, Z = O, S, N, C such that one of W, X, Y, Z = O, S and at least one of W, X, Y, Z = C; A = H, hydrocarbyl, heterocyclyl, halo, NC, F3C, R3O, R3S, R3R3N, R3COR3N, R3O2CR3N, etc. wherein R3, R4 = H, hydrocarbyl, heterocyclyl, R3R4 = C2-6 alkylene; E = bond, C13-4 alkylene; F = substituted heterocyclyl) or a salt thereof, are prepared
 To 5-(aminomethyl)-3-[2-(N-tert-butoxycarbonylamino)ethyl]-14-indole (preparation given) in THF and (Me2CH)2NET was added 5-chloro-3-methyl-1,2,4-

L10 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 thiadiazole to give the protected thiadiazolylamine which in CH2Cl2 was reacted with F3CCO2H to give the title compd. II. The activity of I as agonists of 5-HT1 receptors was measured as to their ability to mediate contraction of the saphenous vein and calcd. as -log10EC50(pEC50) from plots of % 5-HT (1 μM) response against the concn. of the agonist and was not less than 5.0. A tablet formulation comprising I is given.
 IT 152673-51-3P 152673-52-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 {preparation and reaction of, in preparation of 5-HT1 agonists}
 RN 152673-51-3 CAPLUS
 CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



RN 152673-52-4 CAPLUS
 CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-5-formyl-, 1,1-dimethylethyl ester (CA INDEX NAME)



L10 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:152309 CAPLUS

DOCUMENT NUMBER: 134:193415

TITLE: Preparation of heteroannelated pyridines as 5-HT1A receptor ligands

INVENTOR(S): Peglioni, Jean-Louis; Dessinges, Aimee; Poitevin, Christophe; Millan, Mark; Dekeyne, Anne

PATENT ASSIGNEE(S): Adir Et Compagnie, Fr.; Les Laboratoires Servier

SOURCE: Eur. Pat. Appl., 27 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1078928	A1	20010228	EP 2000-402359	20000825
EP 1078928	B1	20040512		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2797874	A1	20010302	FR 1999-10834	19990827
FR 2797874	B1	20020329		
US 6399616	B1	20020604	US 2000-641777	20000818
JP 2001097978	A	20010410	JP 2000-252191	20000823
JP 3602780	B2	20041215		
MX 2000PA08241	A	20020820	MX 2000-PA8241	20000823
CA 2317053	A1	20010227	CA 2000-2317053	20000825
ZA 2000004411	A	20010228	ZA 2000-4411	20000825
CN 1286255	A	20010307	CN 2000-124065	20000825
HU 2000003413	A2	20010730	HU 2000-3413	20000825
HU 2000003413	A3	20031128		
AT 266664	T	20040515	AT 2000-402359	20000825
PT 1078928	T	20040930	PT 2000-402359	20000825
ES 2220359	T3	20041216	ES 2000-402359	20000825
NO 2000004295	A	20010228	NO 2000-4295	20000828
NO 316651	B1	20040322		
BR 2000003848	A	20010403	BR 2000-3848	20000828
AU 765661	B2	20030925	AU 2000-53642	20000828
HK 1034250	A1	20050429	HK 2001-104815	20010711
US 2002161220	A1	20021031	US 2002-105171	20020325
US 6486171	B2	20021126		

PRIORITY APPLN. INFO.: FR 1999-10834 A 19990827

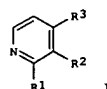
US 2000-641777 A3 20000818

OTHER SOURCE(S): MARPAT 134:193415

GI

L10 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)

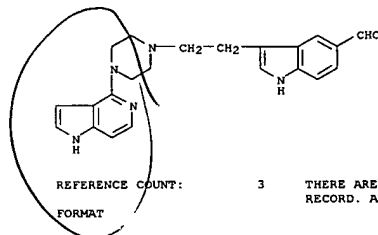


AB Title compds. [I; R1 = R(CH2)nZ1; R = (un)substituted naphthyl or heteroannelated Ph; R2R3 = atoms to complete a thiophene, furan, or (oxo)pyrrole ring; Z = bonds, O, [(ar)alkyl]imino; Z1 = 1,4-cyclohexylene, piperidine-1,4- or -4,1-diyl, piperazine-1,4-diyl; n = 1-6] were prepared. Thus, 7-chlorofuro[2,3-c]pyridine was aminated by N-(2-naphthylmethyl)-4-piperidineamine to give I (R1 = RCH2NHZ1, R = 2-naphthyl, R2R3 = OCH:CH, Z1 = piperidine-4,1-diyl). Data for biol. activity of I were given.

IT 327173-90-OP
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RN 327173-90-0 CAPLUS
(preparation of heteroannelated pyridines as 5-HT1A receptor ligands)

CN 1H-Indole-5-carboxaldehyde, 3-[2-[4-(1H-pyrrolo[3,2-c]pyridin-4-yl)-1-piperazinyl]ethyl]- (CA INDEX NAME)



REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

R³ R⁴ X

L10 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:19828 CAPLUS

DOCUMENT NUMBER: 136:263284

TITLE: The chemistry of indoles. Part 109. Synthetic studies of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position

AUTHOR(S): Yamada, Fumio; Tamura, Mayumi; Hasegawa, Atsuko; Sonei, Masanori

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kanazawa University, Kanazawa, 920-0934, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(1), 92-99

CODEN: CPBTAL; ISSN: 0009-2363

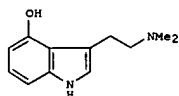
PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:263284

GI



I

AB Psilocin (I) analogs having either a formyl group or a bromine atom at the 5- or 7-position have been prepared for the first time. Syntheses of 5- and 7-bromo derivs. of 4-hydroxy- and 4-benzyloxyindole-3-carbaldehyde, 4-benzyloxyindole-3-acetonitriles, and 4-benzyloxy-N,N-dimethyltryptamine have also been established.

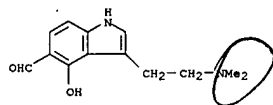
IT 404887-81-6P 404887-83-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position)

RN 404887-81-6 CAPLUS

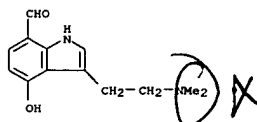
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-4-hydroxy- (CA INDEX NAME)



L10 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 404887-83-8 CAPLUS

CN 1H-Indole-7-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-4-hydroxy- (CA INDEX NAME)



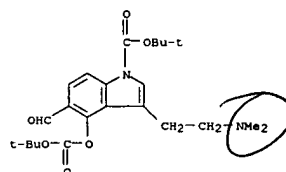
IT 404887-84-9P 404887-85-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position)

RN 404887-84-9 CAPLUS

CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-4-[[[(1,1-dimethylethoxy)carbonyl]oxy]-5-formyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

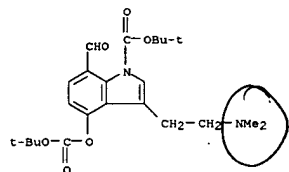


RN 404887-85-0 CAPLUS

CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-4-[[[(1,1-dimethylethoxy)carbonyl]oxy]-7-formyl-, 1,1-dimethylethyl ester (CA INDEX NAME)

L10 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L10 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:546477 CAPLUS

DOCUMENT NUMBER: 141:89009

TITLE: Synthesis of tryptamine derivatives and intermediates thereof

INVENTOR(S): Berens, Ulrich; Dosenbach, Oliver; Sprenger, Daniel

PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.

SOURCE: PCT Int. Appl., 84 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056769	A2	20040708	WO 2003-EP50992	20031212
WO 2004056769	A3	20040916		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,				
TG				
CA 2508290	A1	20040708	CA 2003-2508290	20031212
AU 2003299227	A1	20040714	AU 2003-299227	20031212
EP 1572647	A2	20050914	EP 2003-799560	20031212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, PL, TA, BG, CZ, EE, HU, SK				
CN 1729174	A	20060201	CN 2003-80107086	20031212
JP 2006516128	T	20060622	JP 2004-561492	20031212
US 2006058367	A1	20060316	US 2005-539151	20050616
IN 2005CN01638	A	20070622	IN 2005-CN1638	20050719
PRIORITY APPLN. INFO.:				
EP 2002-406128 A 20021220				
WO 2003-EP50992 W 20031212				

OTHER SOURCE(S): MARPAT 141:89009

GI

L10 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

AB Indoleacetates I [R = CO2R3; R1 = (un)substituted alkyl, aryl, heterocyclyl, alkylsulfonyl, OH, SH, NO2, halogen, CN, CONH2, CONHNH2, CO2H, alkenyl, alkynyl, cycloalkyl, acyloxy, NH2, NHHH2, B(OH)2; R2 = H, (un)substituted alkyl, CO2H, arylsulfonyl, alkylsulfonyl, aryl, CONH2, silyl; R3 = (un)substituted alkyl; n = 0-4] were prepared and converted

to I [R = CONR4R5; R4, R5 = (un)substituted alkyl; R4R5 = (un)substituted alkylene] which were in turn converted to indoleacetamides and tryptamines. The synthesis methods and products are useful in the synthesis of pharmaceuticals. Thus, 5-bromoindole was treated with CH2(CO2H)2 and ClCONMe2 to give I [R = CONMe2, R1 = 5-Br, R2 = H] which was treated with BF3.Et2O and BH3.Me2SO to give

2-[5-bromo-1H-indol-3-yl]-N,N-dimethylacetamide or with BF3.Et2O and NaBH4 to give

[2-[5-bromo-1H-indol-3-yl]ethyl]-N,N-dimethylacetamide.

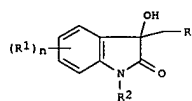
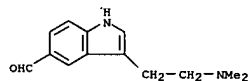
IT 152673-51-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tryptamine derivs. and intermediates thereof)

RN 152673-51-3 CAPLUS

CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (CA INDEX NAME)

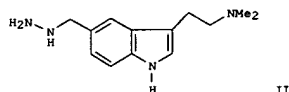
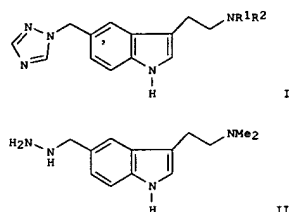


L10 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2005:811739 CAPLUS
 DOCUMENT NUMBER: 143:229863
 TITLE: A manufacturing of (triazolymethyl)indole
 derivatives
 INVENTOR(S): and their intermediates
 Martin, Pierre; Berens, Ulrich; Boudier, Andreas;
 Dosenbach, Oliver
 PATENT ASSIGNEE(S): Ratiopharm G.m.b.H., Germany
 SOURCE: PCT Int. Appl., 67 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005075422	A1	20050818	WO 2005-EP793	20050127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2553652	A1	20050818	CA 2005-2553652	20050127
EP 1751104	A1	20070214	EP 2005-707035	20050127
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
IN 2006DN03983	A	20070824	IN 2006-DN3983	20060711
US 2007123711	A1	20070531	US 2006-586958	20061128
PRIORITY APPL. INFO.:			EP 2004-100303	A 20040128
			US 2004-543463P	P 20040210
			WO 2005-EP793	W 20050127

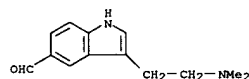
OTHER SOURCE(S): MARPAT 143:229863
 GI

L10 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



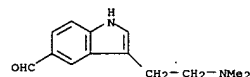
AB The invention relates to a preparation of (triazolymethyl)indole derivs. of formula I [wherein: R1 and R2 are independently H or alkyl] and their intermediates. For instance, anti-migraine agent rizatriptan I [R1 = R2 = Me; no biol. data] was prepared from [(hydrazinomethylindolyl)ethyl]-dimethyl-amine II with a yield of 55%.

IT 152673-51-3P 862703-18-2P 862703-19-3P
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (manufacturing of (triazolymethyl)indole derivs. and their intermediates)
 RN 152673-51-3 CAPLUS
 CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (CA INDEX NAME)



RN 862703-18-2 CAPLUS
 CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L10 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

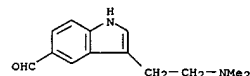


● HCl

RN 862703-19-3 CAPLUS
 CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-, ethanedioate (1:1) (CA INDEX NAME)

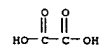
CM 1

CRN 152673-51-3
 CMF C13 H16 N2 O



CM 2

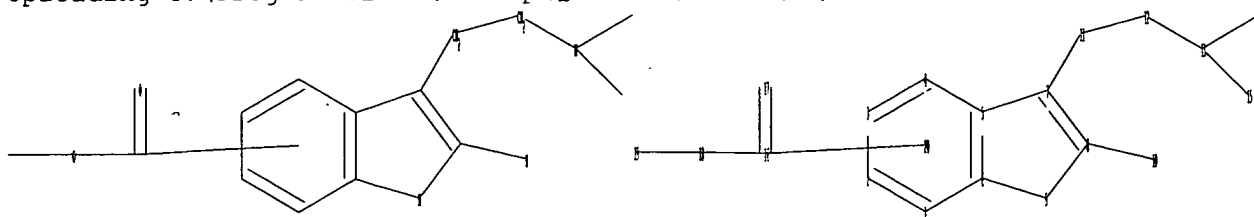
CRN 144-62-7
 CMF C2 H2 O4



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

=>

Uploading C:\Program Files\Stnexp\Queries\10539151\Jan4.str



claim 32

```

chain nodes :
10 11 12 16 17 18
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 14 15 19
chain bonds :
7-11 8-10 11-12 12-13 16-17 16-18 18-19
ring/chain bonds :
13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15 16-17 16-18 18-19
exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

```

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:Atom

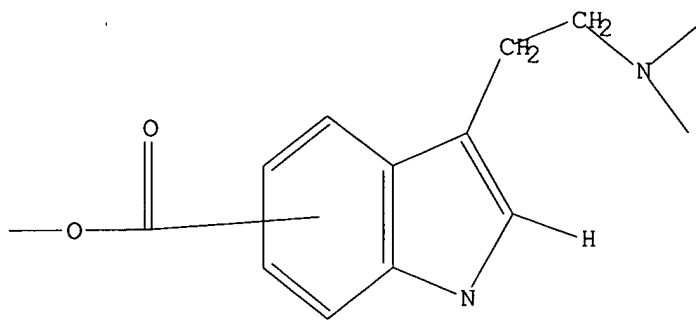
```

L11 STRUCTURE UPLOADED

=> d

L11 HAS NO ANSWERS

L11 STR

*derim 32*

Structure attributes must be viewed using STN Express query preparation.

=> s l11 full sub=l3 ✓

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 11:38:50 FILE 'REGISTRY'

FULL SUBSET SCREEN SEARCH COMPLETED - 5875 TO ITERATE

100.0% PROCESSED 5875 ITERATIONS

SEARCH TIME: 00.00.01

7 ANSWERS ✓

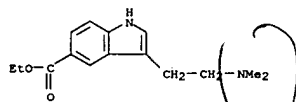
L12 7 SEA SUB=L3 SSS FUL L11

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH

L13 6 L12 ✓

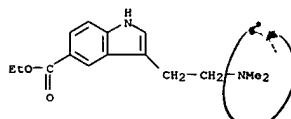
=> d ibib abs hitstr l13 tot

L13 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2003:234500 CAPLUS
 DOCUMENT NUMBER: 139:52822
 TITLE: Synthesis of 3-[2-(dimethylamino)ethyl]-2-[[3-(dimethylamino)ethyl]-1H-indol-5-yl]methyl-1H-indol-5-yl-N-methylmethanesulfonamide - the main sumatriptan impurity
 AUTHOR(S): Skwierawska, A.; Paluszkiwicz, E.
 CORPORATE SOURCE: Department of Chemistry, Gdansk University of Technology, Gdansk, 80-952, Pol.
 SOURCE: Polish Journal of Chemistry (2003), 77(3), 329-332
 CODEN: PJCHDQ; ISSN: 0137-5083.
 PUBLISHER: Polish Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 139:52822
 AB Alkylation of sumatriptan in position 2 by 3-[2-(dimethylamino)ethyl]-5-indolemethanol is described. Alternative multistep synthesis of 3-[2-(dimethylamino)ethyl]-5-indolemethanol is presented.
 IT 137499-21-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of
 3-[2-(dimethylamino)ethyl]-2-[[3-(dimethylamino)ethyl]-1H-indol-5-yl]methyl-1H-indol-5-yl]-N-methylmethanesulfonamide via Fischer indole synthesis)
 RN 137499-21-9 CAPLUS
 CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester
 (CA INDEX NAME)

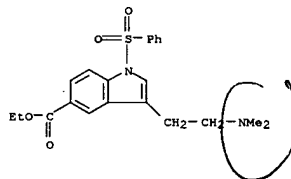


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L13 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2001:83714 CAPLUS
 DOCUMENT NUMBER: 134:311061
 TITLE: Synthesis of 5-(sulfamoylmethyl)indoles
 AUTHOR(S): Bosch, J.; Roca, T.; Armengol, M.; Fernandez-Fornier, D.
 CORPORATE SOURCE: Laboratory of Organic Chemistry, Faculty of Pharmacy, University of Barcelona, Barcelona, 08028, Spain
 SOURCE: Tetrahedron (2001), 57(6), 1041-1048
 CODEN: TETRA; ISSN: 0040-4020
 PUBLISHER: Elsevier Science Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 134:311061
 AB The synthesis of 5-(sulfamoylmethyl)indoles bearing a two-carbon chain at C-3 (aminoethyl, acetate, hydroxyethyl, ethyl) either by the Grandberg modification of the Fischer indolization or by intramol. Heck reaction of suitable o-halo-trifluoroacetanilides is reported.
 IT 137499-21-9P 334981-33-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of 5-(sulfamoylmethyl)indoles)
 RN 137499-21-9 CAPLUS
 CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester
 (CA INDEX NAME)



RN 334981-33-8 CAPLUS
 CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-1-(phenylsulfonyl)-, ethyl ester (CA INDEX NAME)

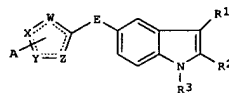


L13 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L13 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1995:610523 CAPLUS
 DOCUMENT NUMBER: 123:9441
 TITLE: Indole-substituted five-membered heteroaromatic compounds as 5-HT1 receptor agonists
 INVENTOR(S): Baker, Raymond; Reeve, Austin J.; Street, Leslie J.
 PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK
 SOURCE: U.S., 31 pp. Cont. of U.S. Ser. No. 641,422, abandoned.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

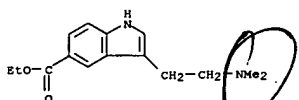
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5317103	A	19940531	US 1992-914683	19920716
PRIORITY APPLN. INFO.:			US 1991-641422	B1 19910115

OTHER SOURCE(S): MARPAT 123:9441
 GI



AB The title compds. (I; A = H, halogen, CN, NO2, CF3, (un)substituted NH2, etc.; E = (un)branched C1-4 alkylene, direct bond; R1 = (un)substituted aminoalkyl, (un)substituted heterocyclyl; R2, R3 = H, C1-6 alkyl, alkenyl, alkynyl; W, X, Y, Z = O, S, N, C; where >1 of W, X, Y, Z = O or S and >1 of W, X, Y, Z = C), useful as specific agonists of 5-HT1-like receptors (no data) and which are useful in the treatment of migraine headache and associated disorders (no data), are prepared and I-containing formulations presented. Thus, 2-[5-[5-(3-benzyl-1,2,4-oxadiazol)-yl]-1H-indol-3-yl]ethylamine hydrogen oxalate hydrate, m.p. 229°, was prepared
 IT 137499-21-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of indole-substituted 5-membered heteroaroms. as 5-HT1 receptor agonists)
 RN 137499-21-9 CAPLUS
 CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester
 (CA INDEX NAME)

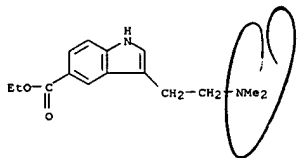
L13 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



IT 163797-85-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of indole-substituted 5-membered heteroaroms. as 5-HT1 receptor agonists)
 RN 163797-85-1 CAPLUS
 CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 137499-21-9
 CMF C15 H20 N2 O2

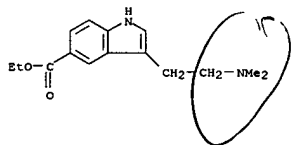


CM 2

CRN 144-62-7
 CMF C2 H2 O4

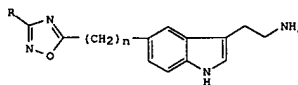


L13 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 functional activity of this series of compds. is studied and demonstrates high 5-HT1D receptor potency and efficacy comparable to that of 5-HT.
 IT 137499-21-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclization of, with amide oximes, oxadiazoles from)
 RN 137499-21-9 CAPLUS
 CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester (CA INDEX NAME)



L13 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:603336 CAPLUS
 DOCUMENT NUMBER: 119:203336
 TITLE: Synthesis and serotonergic activity of 5-(oxadiazolyl)tryptamines: potent agonists for 5-HT1D receptors
 AUTHOR(S): Street, Leslie J.; Baker, Raymond; Castro, Jose L.; Chambers, Mark S.; Guiblin, Alexander R.; Hobbs, Sarah
 C.; Matassa, Victor G.; Reeve, Austin J.; Beer, Margaret S.; et al.
 CORPORATE SOURCE: Chem. Dep., Merck Sharp and Dohme Res. Lab., Harlow/Essex, CM20 2QR, UK
 SOURCE: Journal of Medicinal Chemistry (1993), 36(11), 1529-38
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



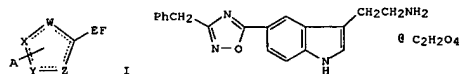
AB The synthesis and 5-HT1D receptor activity of a novel series of 5-(oxadiazolyl)tryptamines I (R = Me, Et, H2N, Ph, PhCH2, 4-MeSO2NHC6H4CH2, etc.; n = 0-3) is described. Modifications of the oxadiazole 3-substituent, length of the linking chain (n), and the amine substituents are explored and reveal a large binding pocket in the 5-HT1D receptor domain. Oxadiazole substituents such as benzyl are accommodated without loss of agonist potency or efficacy. The incorporation of polar functionality on a Ph or benzyl spacer group results in a 10-fold increase in affinity and functional potency. Optimal 5-HT1D activity is observed when the heterocycle is conjugated with the indole and the benzyl sulfonamides represent some of the most potent 5-HT1D agonists known. Replacement of O for S in the heterocycle leads to a further increase in potency. Deletion of oxadiazole N-2 does not reduce activity, suggesting the requirement for only one H-bond acceptor in this location. The selectivity of these compds. for 5-HT1D receptors over other serotonergic receptors is discussed. Sulfonamide I (R = 4-MeSO2NHC6H4CH2, n = 0) shows >1000-fold selectivity for 5-HT1D over 5-HT2, 5-HT1C, and 5-HT3 receptors and 10-fold selectivity with respect to 5-HT1A receptors. The

L13 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:83677 CAPLUS
 DOCUMENT NUMBER: 116:83677
 TITLE: Preparation of substituted (1,2,4-oxadiazolylindolyl)ethylamine and analogs as agonists of 5-HT1-like receptors
 INVENTOR(S): Baker, Raymond; Reeve, Austin J.; Street, Leslie J.
 PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK
 SOURCE: Eur. Pat. Appl., 58 pp.
 CODEN: EPXXEW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 438230	A2	19910724	EP 1991-300180	19910110
EP 438230	A3	19920212		
EP 438230	B1	19970423		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 152110	T	19970515	AT 1991-300180	19910110
CA 2034189	A1	19910718	CA 1991-2034189	19910115
FI 9100228	A	19910718	FI 1991-228	19910116
NO 9100187	A	19910718	NO 1991-187	19910116
AU 9169440	A	19910725	AU 1991-69440	19910116
CN 1053429	A	19910731	CN 1991-100380	19910117
JP 06100558	A	19940412	JP 1991-216736	19910117
PRIORITY APPL. INFO.:				
			GB 1990-1018	A 19900117
			GB 1990-8587	A 19900417

OTHER SOURCE(S): MARPAT 116:83677
 GI

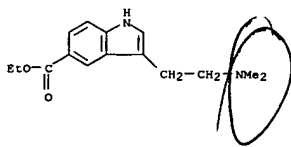


AB Title compds. I [wherein the broken circle represents 2 non-adjacent double bonds in any position; W, X, Y, Z = O, S, N, C, such that 1 of W, X, Y, Z = O, S and at least 1 of W, X, Y, Z = C; A = H, hydrocarbyl, halo, NC, F3C, O2N, etc.; E = bond, C1-4 alkylene, F = (substituted) heterocyclyl] or a salt or prodrug thereof, are prepared NaNO2 was added to 4-(H2N)C6H4CO2Et in concentrated HCl, the mixture stirred at 0° before adding 3nCl2.2H2O in HCl to give 4-(H2NNH)C6H4CO2Et.HCl (II). II and 4-ClCH2(CH2)2CH(OMe)2 in EtOH/H2O were refluxed, the solvent removed and the residue chromatographed to give 2-(5-(5-carbomethoxy-1H-indol-3-yl)ethylamine.H maleate (III). NaH was added to phenylacetamide oxime in THF, the reaction mixture refluxed, III was added and the whole refluxed for 2 h, the reaction mixture cooled to room temperature to give the title compound as

L13 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 the H.oxalate (IV). The activity as agonist of 5-HT₁-like receptor was measured in terms of their ability to mediate contraction of the saphenous vein of rabbits, and the potency calcd. as -log₁₀EC₅₀ (pEC₅₀). The pEC₅₀ of IV was not less than 5.0. Tablet compns. comprising I are given.

IT 137499-21-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, in preparation of 5-HT₁ agonists)

RN 137499-21-9 CAPLUS
 CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester
 (CA INDEX NAME)



L13 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1980:532369 CAPLUS
 DOCUMENT NUMBER: 93:132369
 ORIGINAL REFERENCE NO.: 93:21105A, 21108A
 TITLE: Indole compounds and pharmaceutical compositions containing them

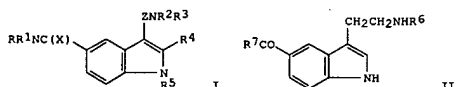
INVENTOR(S): Webb, Colin Frederick
 PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
 SOURCE: Ger. Offen. 102 pp.
 CODEN: GWXXBX

DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2940687	A1	19800430	DE 1979-2940687	19791008
DE 2940687	C2	19910801		
ZA 7905239	A	19801126	ZA 1979-5239	19791002
FI 7903071	A	19800413	FI 1979-3071	19791004
DK 7904255	A	19800413	DK 1979-4255	19791009
AU 7951657	A	19800417	AU 1979-51657	19791010
AU 531783	B2	19830908		
GB 2035310	A	19800618	GB 1979-35208	19791010
GB 2035310	B	19821222		
US 4252803	A	19810224	US 1979-83343	19791010
AT 7906605	A	19840815	AT 1979-6605	19791010
AT 377511	B	19850325		
SE 7908443	A	19800413	SE 1979-8443	19791011
SE 448628	B	19870309		
SE 448628	C	19870618		
CH 646151	A5	19841115	CH 1979-9194	19791011
BE 879381	A1	19800201	BE 1979-197621	19791012
NL 7907583	A	19800415	NL 1979-7583	19791012
FR 2438651	A1	19800509	FR 1979-25446	19791012
FR 2438651	B1	19830304		
JP 55062063	A	19800510	JP 1979-130944	19791012
JP 63058817	B	19881117		
CA 1146550	A1	19830517	CA 1979-337443	19791012
ES 485830	A5	19801030	ES 1979-485830	19791108
PRIORITY APPLN. INFO.:				GB 1978-40279 A 19781012
				JP 1978-138402 A 19781111
				JP 1979-73064 A 19790612

OTHER SOURCE(S): MARPAT 93:132369
 GI

L13 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



AB The indole derivs. I [R, R₁, R₂, R₃ = H, (substituted) alkyl, cycloalkyl, aryl, or aralkyl; RR₁N, and R₂R₃N = ring; R₄ = H, C1-3 alkyl, aryl; R₅ = H, alkyl, aralkyl; Z = C1-4 alkylene; X = O, S] and their salts were prepared for use in treatment of hypertension and migraines (no data). Thus, II (R₆ = CO₂CH₂Ph, R₇ = OH) reacted with PhCH₂NH₂ in the presence

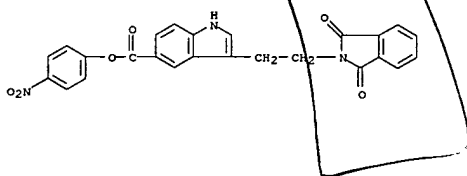
of 2-chloro-1-methylpyridinium iodide to give II (R₆ = CO₂CH₂Ph, R₇ = NHCH₂Ph), which was hydrogenated over Pd-C to give I (R₆ = H, R₇ = NHCH₂Ph), isolated as compound with creatinine sulfate.

IT 74884-82-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and amidation of)

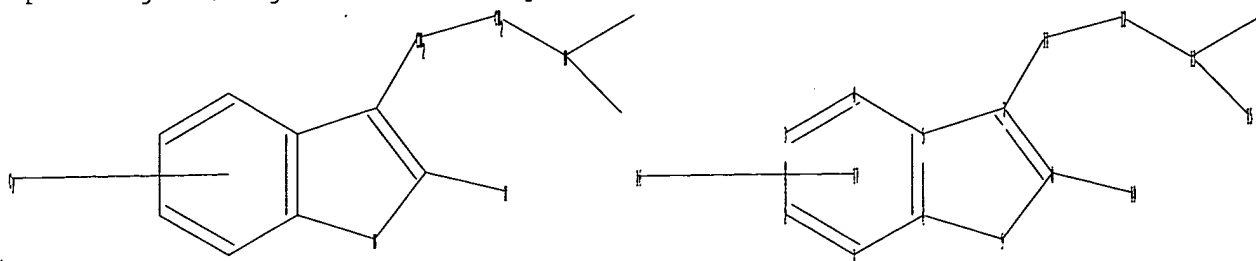
RN 74884-82-5 CAPLUS

CN 1H-Indole-5-carboxylic acid, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-, 4-nitrophenyl ester (CA INDEX NAME)



=>

Uploading C:\Program Files\Stnexp\Queries\10539151\Jan5.str



```

chain nodes :
10 11 12 16
ring nodes :
1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 14 15
chain bonds :
7-11 8-10 11-12 12-13
ring/chain bonds :
13-14 13-15
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-14 13-15
exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

```

Match level :

```

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:Atom

```

Generic attributes :

16:

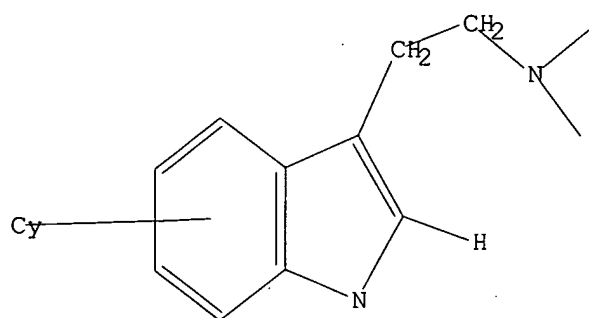
Saturation : Unsaturated

L14 STRUCTURE UPLOADED

=> d

L14 HAS NO ANSWERS

L14 STR



claim 4/
(XIV')

Structure attributes must be viewed using STN Express query preparation.

=> s l14 full sub=l3

REGISTRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress...

Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SUBSET SEARCH INITIATED 11:42:05 FILE 'REGISTRY'
FULL SUBSET SCREEN SEARCH COMPLETED - 5875 TO ITERATE

100.0% PROCESSED 5875 ITERATIONS
SEARCH TIME: 00.00.01

26 ANSWERS ✓

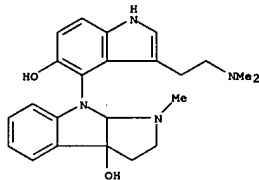
L15 26 SEA SUB=L3 SSS FUL L14

SUBSET IS IGNORED AS A SCOPE FOR THIS SEARCH
L16 11 L15

=> d ibib abs hitstr l16 tot ✓

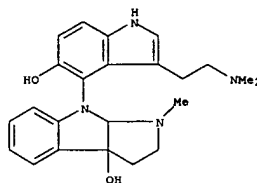
L16 ANSWER 1 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:692189 CAPLUS
 DOCUMENT NUMBER: 142:236417
 TITLE: Alkaloids from Arundo donax. XVI. Structure of the New
 AUTHOR(S): Dimeric Indole Alkaloid Arundavine
 Khuzhaev, V. U.; Zhalolov, I.; Turgunov, K. K.;
 Tashkhodzhaev, B.; Levkovich, M. G.; Aripova, S. F.;
 Shashkov, A. S.
 CORPORATE SOURCE: Kokand State Pedagogical Institute, Uzbekistan
 SOURCE: Chemistry of Natural Compounds (Translation of
 Khimiya Prirodnykh Soedinenii) (2004), 40(3), 261-265
 CODEN: CHNCAS; ISSN: 0009-3130
 PUBLISHER: Kluwer Academic/Consultants Bureau
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The new bis-indole alkaloid arundavine, a tryptamine-tryptamine base, was isolated from roots of Arundo donax. The dimer consists of monomeric units of two known indole alkaloids, alline and bufotenine, joined through the N1 and C4' atoms, resp., to give the structure 8-[3-(2-dimethylaminoethyl)-5-hydroxy-1H-indol-4-yl]-1-methyl-2,3,8a-tetrahydro-1H-pyrrolo[2,3-b]indol-3a-ol.
 IT 844696-24-8, Arundavine
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); BIOL (Biological study); OCCU (Occurrence) (structure of new dimeric indole alkaloid arundavine)
 RN 844696-24-8 CAPLUS
 CN Pyrrolo[2,3-b]indol-3a(1H)-ol, 8-[3-(2-(dimethylamino)ethyl)-5-hydroxy-1H-indol-4-yl]-2,3,8a-tetrahydro-1-methyl- (CA INDEX NAME)

Currently available stereo shown.



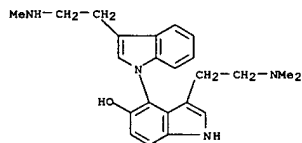
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L16 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:541463 CAPLUS
 DOCUMENT NUMBER: 142:236397
 TITLE: Alkaloids of the flora of Uzbekistan, Arundo donax
 AUTHOR(S): Khuzhaev, V. U.
 CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant Substances, Tashkent and Kokand State Pedagogic Institute, Academy of Sciences of the Republic of Uzbekistan, Kokand, Uzbekistan
 SOURCE: Chemistry of Natural Compounds (Translation of
 Khimiya Prirodnykh Soedinenii) (2004), 40(2), 160-162
 CODEN: CHNCAS; ISSN: 0009-3130
 PUBLISHER: Kluwer Academic/Consultants Bureau
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Alkaloids of Arundo donax L. growing in four soil-climatic regions of Uzbekistan were studied. Twenty alkaloids, including the new ones arundavine and arundanine, were isolated from the plant.
 IT 844696-24-8P, Arundavine
 RL: NPO (Natural product occurrence); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation) (new alkaloids isolated from Arundo donax)
 RN 844696-24-8 CAPLUS
 CN Pyrrolo[2,3-b]indol-3a(1H)-ol, 8-[3-(2-(dimethylamino)ethyl)-5-hydroxy-1H-indol-4-yl]-2,3,8a-tetrahydro-1-methyl- (CA INDEX NAME)
 Currently available stereo shown.

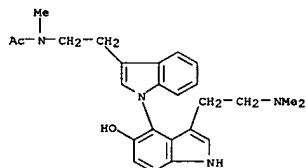


IT 475977-53-8, Arundamine 492994-31-7, Arundanine
 618852-71-4, Arundanine
 RL: BSU (Biological study, unclassified); BIOL (Biological study) (of Arundo donax growing in Uzbekistan)
 RN 475977-53-8 CAPLUS
 CN [1,4'-Bi-1H-indol]-5'-ol, 3'-[2-(dimethylamino)ethyl]-3-[2-(methylamino)ethyl]- (CA INDEX NAME)

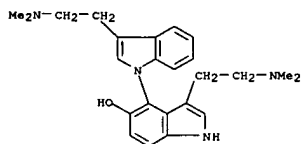
L16 ANSWER 2 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 492994-31-7 CAPLUS
 CN Acetamide, N-[2-[3'-(2-(dimethylamino)ethyl)-5'-hydroxy[1,4'-bi-1H-indol]-3-yl]ethyl]-N-methyl- (CA INDEX NAME)

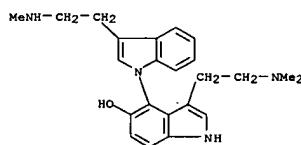


RN 618852-71-4 CAPLUS
 CN [1,4'-Bi-1H-indol]-5'-ol, 3,3'-bis[2-(dimethylamino)ethyl]- (CA INDEX NAME)



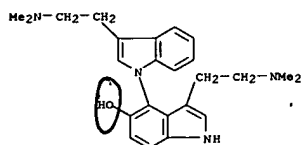
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

L16 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 2004:541433 CAPLUS
 DOCUMENT NUMBER: 142:156195
 TITLE: Alkaloids from Arundo donax L. X. Mass spectrometric fragmentation of Arundamine and Arundanine
 AUTHOR(S): Khuzhaev, V. U.
 CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan
 SOURCE: Chemistry of Natural Compounds (Translation of
 Khimiya Prirodnykh Soedinenii) (2004), 40(2), 196-197
 CODEN: CHNCAS; ISSN: 0009-3130
 PUBLISHER: Kluwer Academic/Consultants Bureau
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The mass spectrometric fragmentation of arundamine (1) and arundanine (2) isolated from Arundo donax was studied in light of the structures established for them. The compds. differ in ion mol. weight by 14 amu. Therefore, the fragmentation of these compds. is observed to be completely parallel. Thus, elimination from the side chains of a C2H6N fragment produces strong peaks with m/z 332 (for 1) and 346 (for 2). Loss of a C3H8N fragment (58 amu) in turn leads to ions with m/z 318 (1) and 332 (2), resp. Loss of the side chains in both instances gives rise to peaks with m/z of 273 and 259. Elimination of fragments of 28 amu converts them to ions with m/z 245 and 231, resp.
 IT 475977-53-8, Arundamine 618852-71-4, Arundanine
 RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study) (mass spectrometric fragmentation of arundamine and arundanine, alkaloids from Arundo donax)
 RN 475977-53-8 CAPLUS
 CN [1,4'-Bi-1H-indol]-5'-ol, 3'-[2-(dimethylamino)ethyl]-3-[2-(methylamino)ethyl]- (CA INDEX NAME)



RN 618852-71-4 CAPLUS
 CN [1,4'-Bi-1H-indol]-5'-ol, 3,3'-bis[2-(dimethylamino)ethyl]- (CA INDEX NAME)

L16 ANSWER 3 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L16 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

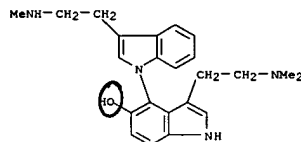
ACCESSION NUMBER: 2003:56668 CAPLUS
 DOCUMENT NUMBER: 139:348106
 TITLE: Alkaloids of Arundo donax L. 13. The structure of a new dimeric indole alkaloid, arundanine
 AUTHOR(S): Khuzhaev, V. U.; Zhalolov, I. Zh.; Levkovich, M. G.; Aripova, S. F.
 CORPORATE SOURCE: Kokand State Pedagogical Institute, Kokand, Uzbekistan
 SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (2003), 52(3), 745-747
 CODEN: RCBUEY; ISSN: 1066-5285
 PUBLISHER: Kluwer Academic/Consultants Bureau
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The structure of a new dimeric indole alkaloid, named arundanine (I), isolated from the roots of Arundo donax L. (Poaceae), was elucidated. I was identified as 3-(N,N-dimethylaminoethyl)-4-[3-(N,N-dimethylaminoethyl)indole-1-yl]-5-hydroxyindole on the basis of spectroscopic data and the transformation into the known alkaloid, arundamine (II).

IT 475977-53-8, Arundamine
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (new dimeric indole alkaloid arundanine of Arundo donax transformation to arundamine)

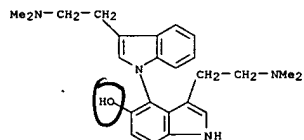
RN 475977-53-8 CAPLUS
 CN [1,4'-Bi-1H-indol]-5'-ol, 3'-[2-(dimethylamino)ethyl]-3-[2-(methylamino)ethyl]- (CA INDEX NAME)



IT 618852-71-4P, Arundanine
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); RCT (Reactant); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); RACT (Reactant or reagent)
 (structure of new dimeric indole alkaloid arundanine of Arundo donax)

L16 ANSWER 4 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 618852-71-4 CAPLUS
 CN [1,4'-Bi-1H-indol]-5'-ol, 3,3'-bis[2-(dimethylamino)ethyl]- (CA INDEX NAME)

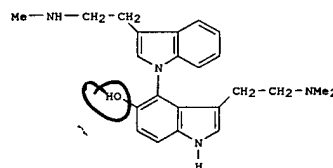


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L16 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

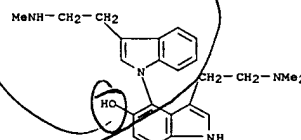
ACCESSION NUMBER: 2002:795021 CAPLUS
 DOCUMENT NUMBER: 137:382263
 TITLE: Alkaloids of Arundo donax. IX. Crystal structure of arundamine
 AUTHOR(S): Zhalolov, I. Zh.; Tashkhodzhaev, B.; Khuzhaev, V. U.; Aripova, S. F.
 CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan
 SOURCE: Chemistry of Natural Compounds (Translation of Khimiya Prirodnikh Soedinenii) (2002), 38(1), 83-86
 CODEN: CHNCAS; ISSN: 0009-3130
 PUBLISHER: Kluwer Academic/Consultants Bureau
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB An x-ray structure anal. was performed for the new dimeric alkaloid arundamine (I) isolated from Arundo donax. Its properties are reported.

IT 475977-53-8P, Arundamine
 RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (crystal structure of arundamine from Arundo donax)

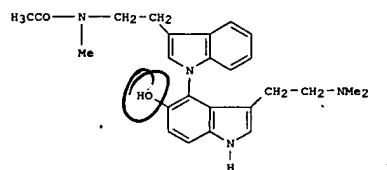
RN 475977-53-8 CAPLUS
 CN [1,4'-Bi-1H-indol]-5'-ol, 3'-[2-(dimethylamino)ethyl]-3-[2-(methylamino)ethyl]- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS

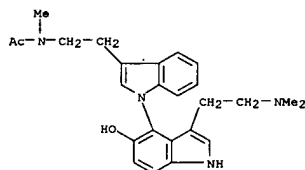
L16 ANSWER 5 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L16 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:750364 CAPLUS
DOCUMENT NUMBER: 138:133835
TITLE: Alkaloids of Arundo donax. XII. Structure of the new dimeric indole alkaloid arundacine
AUTHOR(S): Khuzhaev, V. U.; Zhalolov, I. Zh.; Levkovich, M. G.; Aripova, S. F.; Shashkov, A. S.
CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan
SOURCE: Chemistry of Natural Compounds (Translation of Khimiya Prirodnikh Soedinenii) (2002), 38(3), 280-283
CODEN: CHNCAS; ISSN: 0009-3130
PUBLISHER: Kluwer Academic/Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



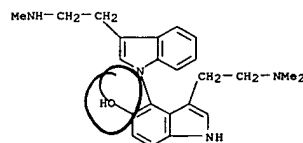
AB The new dimeric indole alkaloid arundacine (I) was isolated from the polar fraction of the total alkaloids from Arundo donax L. roots. The structure
3-N,N-dimethylaminoethyl-5-hydroxy-4-(3'-N'-acetyl-N'-methylaminoethylindol-1'-yl)indole was established using spectral data (IR, UV, mass, one-dimensional ¹H and ¹³C NMR, various two-dimensional spectra).
IT 492994-31-7P, Arundacine
RL: NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
(dimeric indole alkaloid from Arundo donax)
RN 492994-31-7 CAPLUS
CN Acetamide,
N-[2-[3'-[2-(dimethylamino)ethyl]-5'-hydroxy[1,4'-bi-1H-indol]-3-yl]ethyl]-N-methyl- (CA INDEX NAME)

L16 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L16 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:750363 CAPLUS
DOCUMENT NUMBER: 138:137449
TITLE: Alkaloids of Arundo donax. XI. NMR spectroscopic study
AUTHOR(S): Zhalolov, I. Zh.; Khuzhaev, V. U.; Levkovich, M. G.; Aripova, S. F.; Shashkov, A. S.
CORPORATE SOURCE: S. Yu. Yunusov Institute of the Chemistry of Plant Substances, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan
SOURCE: Chemistry of Natural Compounds (Translation of Khimiya Prirodnikh Soedinenii) (2002), 38(3), 276-279
CODEN: CHNCAS; ISSN: 0009-3130
PUBLISHER: Kluwer Academic/Consultants Bureau
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The dimeric indole alkaloid arundamine was isolated from the total bases of Arundo donax L. (Poaceae) roots. The structure of arundamine was investigated using ordinary one-dimensional ¹H and ¹³C NMR, J-modulated ¹³C NMR, and various types of two-dimensional spectra, COSY, NOESY, HSQC, and HMQC.
IT 475977-53-8, Arundamine
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(NMR spectroscopic study of structure of dimeric alkaloid arundamine)
RN 475977-53-8 CAPLUS
CN [1,4'-Bi-1H-indol]-5'-ol, 3'-[2-(dimethylamino)ethyl]-3-[2-(methylamino)ethyl]- (CA INDEX NAME)



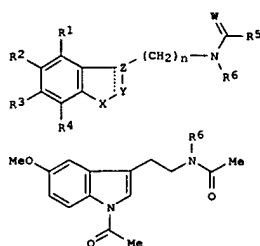
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L16 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN
 ACCESSION NUMBER: 1997:247954 CAPLUS
 DOCUMENT NUMBER: 126:225161
 TITLE: Acylated derivatives of melatonin and its analogs, useful as medicaments
 INVENTOR(S): Fourtillan, Jean-Bernard; Fourtillan, Marianne; Jacquesy, Jean-Claude; Jouannetaud, Marie-Paule; Violeau, Bruno; Karam, Omar
 PATENT ASSIGNEE(S): Cemaf, Fr.; Laboratoires Besins Iscovesco S.A.; Fourtillan, Jean-Bernard; Fourtillan, Marianne; Jacquesy, Jean-Claude; Jouannetaud, Marie-Paule; Violeau, Bruno; Karam, Omar
 SOURCE: PCT Int. Appl., 33 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: French
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9706140	A1	19970220	WO 1996-FR1260	19960807
W: AL, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IS, JP, KP, KR, LK, LR, LT, LV, MG, MK, MN, MW, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
FR 2737725	A1	19970214	FR 1995-9611	19950808
FR 2737725	B1	19971031		
AU 9668236	A	19970305	AU 1996-68236	19960807
EP 851855	A1	19980708	EP 1996-928490	19960807
EP 851855	B1	20020605		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1196049	A	19981014	CN 1996-196943	19960807
CN 1118451	B	20030820		
JP 11510804	T	19990921	JP 1996-508184	19960807
AT 218547	T	20020615	AT 1996-928490	19960807
PT 851855	T	20021031	PT 1996-928490	19960807
ES 2176480	T3	20021201	ES 1996-928490	19960807
ZA 9606751	A	19971103	ZA 1996-6751	19960808
US 6004991	A	19981221	US 1998-11042	19980327
US 6140372	A	20001031	US 1999-292968	19990416
PRIORITY APPLN. INFO.:			FR 1995-9611	A 19950808
			WO 1996-FR1260	W 19960807

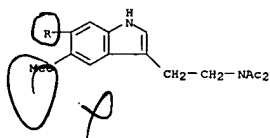
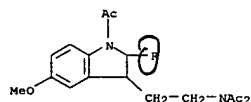
OTHER SOURCE(S): CASREACT 126:225161; MARPAT 126:225161
 GI

L16 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



AB Title derivs. I [W = O, S, (un)substituted NH; X = (un)substituted NH, CH:CH, CH2CH2; YZ = CH:C, C(W)CH, CH2CH; or XYZ = (un)substituted CH2CH:CHCH, CH2C(W)CH2CH, CH2CH2C(W)CH; n = 1-4, especially 2; R1-R6 = H, OH, (un)substituted alk(en/yn)yl, cycloalkyl, alkoxy, aryloxy, aralkoxy, alkylthio, halo, NO2, aryl, etc.), are disclosed, as is a method for their preparation, their therapeutic use, particularly for treating diseases associated with melatonin disorders, and pharmaceutical and cosmetic compns. containing them. For example, treatment of melatonin with NaH in THF, followed by acetyl chloride, gave title compds. II [R6 = H and Ac]. Tests in fish showed that I have a hypnotic effect greater than that of melatonin, and equivalent to that of diazepam.
 IT 188397-12-8P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of acylated melatonin derivs. as drugs and cosmetics)
 RN 188397-12-8 CAPLUS
 CN Acetamide, N,N'-[(1-acetyl-2,3-dihydro-5,5'-dimethoxy[2,6'-bi-1H-indole]-3,3'-diyl)di-2,1-ethanediy]bis[N-acetyl- (9CI) (CA INDEX NAME)]

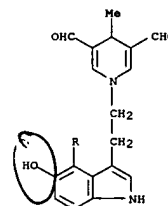
L16 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



L16 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:774512 CAPLUS
 DOCUMENT NUMBER: 123:339506
 TITLE: Reaction of malondialdehyde with amine neurotransmitters. Formation and oxidation chemistry of fluorescent 1,4-dihydropyridine adducts
 AUTHOR(S): d'Iachia, Marco; Napolitano, Alessandra; Costantini, Claudio
 CORPORATE SOURCE: Department Organic Biological Chemistry, University Naples Federico II, Naples, I-80134, Italy
 SOURCE: Tetrahedron (1995), 51(34), 9501-8
 CODEN: TETRA8; ISSN: 0040-4020
 PUBLISHER: Elsevier
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Under physiol. relevant conditions, malondialdehyde reacts smoothly with amine neurotransmitters, i.e. dopamine, norepinephrine and serotonin, to give fluorescent dihydropyridines as the relatively most abundant products. Small amts. of enamine derivs. could also be obtained in the reactions with dopamine and serotonin. Oxidation of 1-[2-(3,4-dihydroxyphenyl)ethyl]-4-methyl-1,4-dihydro-3,5-pyridinedicarboxaldehyde with hydrogen peroxide/peroxidase leads to a complex pattern of unstable products, the major of which has been isolated and identified as a o-quinone epoxide. Similar oxidation of the other dihydropyridines affords mainly the N-unsubstituted dihydropyridine and the 4,4'-biindolyl derivative, resp. These results provide new clues to the role of malondialdehyde in neuronal degeneration and lipofuscin formation.
 IT 170803-42-6P
 RL: BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation) (1,4-dihydropyridine adducts from malondialdehyde and neurotransmitter amines)
 RN 170803-42-6 CAPLUS
 CN 3,5-Pyridinedicarboxaldehyde, 1,1'-[(5,5'-dihydroxy[4,4'-bi-1H-indole]-3,3'-diyl)di-2,1-ethanediy]bis[1,4-dihydro-4-methyl- (9CI) (CA INDEX NAME)]

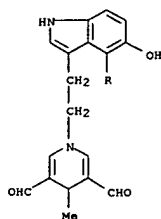
PAGE 1-A



L16 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued)

PAGE 2-A

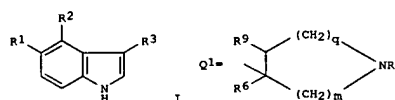


L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

1995:557092 CAPLUS
 ACCESSION NUMBER: 122:290709
 DOCUMENT NUMBER: Preparation of tryptamine analogs as 5-HT1-like agonists or partial agonists.
 TITLE: Porter, Roderick Alan; Coates, William John
 INVENTOR(S): SmithKline Beecham PLC, UK
 PATENT ASSIGNEE(S): PCT Int. Appl., 43 pp.
 SOURCE: CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9414771	A1	19940707	WO 1993-EP3564	19931214
M: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, LV, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9458119	A	19940719	AU 1994-58119	19931214
EP 674620	A1	19951004	EP 1994-903794	19931214
R: BE, CH, DE, ES, FR, GB, IT, LI, NL				
JP 08504786	T	19960521	JP 1993-514774	19931214
ZA 9309456	A	19950619	ZA 1993-9456	19931217
CN 1092765	A	19940928	CN 1993-112761	19931220
PRIORITY APPLN. INFO.:				GB 1992-26537 A 19921221
				WO 1993-EP3564 W 19931214

OTHER SOURCE(S): MARPAT 122:290709
 GI



AB Title compds. [I; R1 = (substituted) 6-10-membered (hetero)aryl ring; R2 = H, halo, C1-4 alkyl, CN, NO2, CF3; R3 = CR4R5CH2NR6R7, CH:NNHC(NH)NH2, Q1: R4-R7 = H, C1-4 alkyl; NR6R7 = ring; R8 = H, C1-4 alkyl, C3-6 alkenyl; Ra = H; Rb = H, OH; RaRb = bond; q, m = 1, 2], were prepared I are 5-HT1-like agonists or partial agonists and may be useful in the treatment and/or prophylaxis of migraine, cluster headache, headache associated with vascular

L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
 disorders and other neuralgia. They are also expected to have utility in the treatment or prophylaxis of portal hypertension. Thus, 2-chloro-6-nitro-3-phenyltoluene (prepn. given) was heated with DMF di-Me acetal and pyrrolidine in DMF at 120°; the resulting enamine was stirred with N2H4 and Raney Ni in MeOH to give 4-chloro-5-phenylindole. This was stirred with AcCl and bis(dimethylamino)methane in CH2Cl2 to

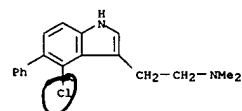
give a residue which was stirred with KCN and MeI in DMF to give 4-chloro-3-cyanomethyl-5-phenylindole. The latter in MeOH was shaken

with Me2NH and Raney Ni under 40 psi H to give 4-chloro-3-[2-N,N-(dimethylamino)ethyl]-5-phenylindole. I showed EC50 = 0.03-1.5 µM in the rabbit basilar artery 5-HT1-like receptor screen.

IT 163104-46-9P 163104-47-0P 163104-66-3P
 163104-70-9P 163104-71-0P 163104-85-6P
 163104-86-7P 163104-89-0P 163104-90-3P
 163105-04-2P 163105-07-5P 163105-08-6P
 163105-11-1P 163105-26-8P 163105-27-9P
 163105-29-1P 163105-95-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of tryptamine analogs as 5-HT1-like agonists or partial agonists)

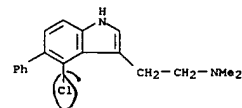
RN 163104-46-9 CAPLUS
 CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-phenyl- (CA INDEX NAME)



RN 163104-47-0 CAPLUS
 CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-phenyl-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 163104-46-9
 CMF C18 H19 Cl N2



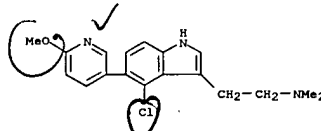
CM 2

L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

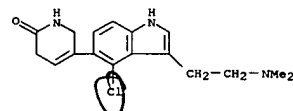
CRN 144-62-7
 CMF C2 H2 O4



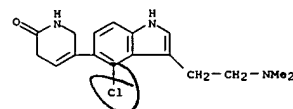
RN 163104-66-3 CAPLUS
 CN 1H-Indole-3-ethanamine, 4-chloro-5-(6-methoxy-3-pyridinyl)-N,N-dimethyl- (CA INDEX NAME)



RN 163104-70-9 CAPLUS
 CN 2(1H)-Pyridinone, 5-[4-chloro-3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]-3,6-dihydro-, monohydrate (9CI) (CA INDEX NAME)



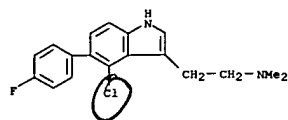
RN 163104-71-0 CAPLUS
 CN 2(1H)-Pyridinone, 5-[4-chloro-3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]-3,6-dihydro-, monohydrate (9CI) (CA INDEX NAME)



● HI

RN 163104-85-6 CAPLUS
 CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-fluorophenyl)-N,N-dimethyl- (CA INDEX NAME)

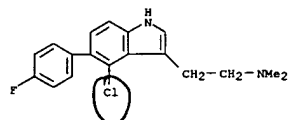
L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 163104-86-7 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-fluorophenyl)-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 163104-85-6
CMF C18 H18 Cl F N2

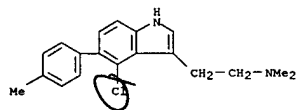


CM 2

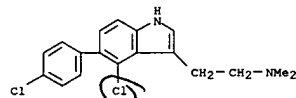
CRN 144-62-7
CMF C2 H2 O4



RN 163104-89-0 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-(4-methylphenyl)- (CA INDEX NAME)



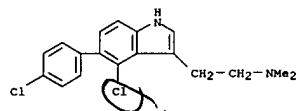
L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 163105-08-6 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-chlorophenyl)-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 163105-07-5
CMF C18 H18 Cl2 N2

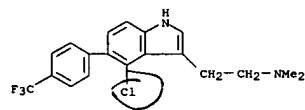


CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 163105-11-1 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



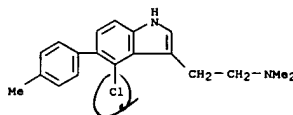
RN 163105-26-8 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(2-methoxy-3-pyridinyl)-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)

L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 163104-90-3 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-N,N-dimethyl-5-(4-methylphenyl)-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 163104-89-0
CMF C19 H21 Cl N2

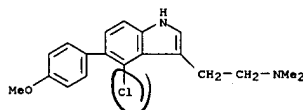


CM 2

CRN 144-62-7
CMF C2 H2 O4

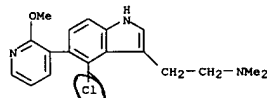


RN 163105-04-2 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-methoxyphenyl)-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)

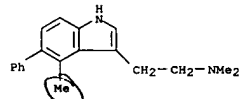


RN 163105-07-5 CAPLUS
CN 1H-Indole-3-ethanamine, 4-chloro-5-(4-chlorophenyl)-N,N-dimethyl-, ethanedioate (9CI) (CA INDEX NAME)

L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



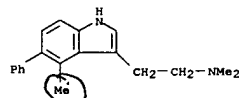
RN 163105-27-9 CAPLUS
CN 1H-Indole-3-ethanamine, N,N,4-trimethyl-5-phenyl-, ethanedioate (9CI) (CA INDEX NAME)



RN 163105-29-1 CAPLUS
CN 1H-Indole-3-ethanamine, N,N,4-trimethyl-5-phenyl-, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 163105-27-9
CMF C19 H22 N2



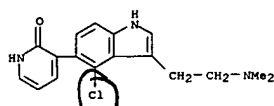
CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 163105-95-1 CAPLUS
CN 2(1H)-Pyridinone, 3-[4-chloro-3-[2-(dimethylamino)ethyl]-1H-indol-5-yl]- (CA INDEX NAME)

L16 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

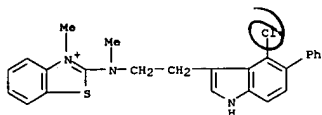


IT 163105-78-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of tryptamine analogs as 5-HT1-like agonists or partial agonists)
 RN 163105-78-0 CAPLUS
 CN Benzothiazolium,
 2-[(2-(4-chloro-5-phenyl-1H-indol-3-yl)ethyl)methylamino]-
 3-methyl-, salt with 4-methylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 163105-77-9

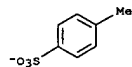
CMF C25 H23 Cl N3 S



CM 2

CRN 16722-51-3

CMF C7 H7 O3 S



L16 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1979:187197 CAPLUS

DOCUMENT NUMBER: 90:187197

ORIGINAL REFERENCE NO.: 90:29756h,29757a

TITLE: Quadrigemines-A and -B, two minor alkaloids of
 Hodgkinsonia frutescens F. Muell
 AUTHOR(S): Parry, Keith P.; Smith, George F.
 CORPORATE SOURCE: Dep. Chem., Univ. Manchester, Manchester, UK
 SOURCE: Journal of the Chemical Society, Perkin Transactions
 1: Organic and Bio-Organic Chemistry (1972-1999)
 (1978), (12), 1671-82
 CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The structures of quadrigemines A (an approx. 1:1 mixture of diastereoisomer I and one (or a mixture of both) of the meso diastereoisomers) and B (II), isolated from *H. frutescens* leaves, were determined by spectroscopic and chemical means. These are the 1st examples of alkaloid structures made up of 4 tryptamine units.

IT 69937-12-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 69937-12-8 CAPLUS

CN [3,7'-Bi-1H-indole]-3,3'-(2H)-diethanamine, N,N,N',N'-tetramethyl-5,5'-
 dinitro- (9CI) (CA INDEX NAME)

